Simulation of dispersion in a heterogeneous aquifer: discussion of steady versus unsteady groundwater flow and an uncertainty analysis

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ABSTRACT: A random walk particle method has been used to simulate the dispersion process of a highly heterogeneous aquifer at Columbus Air Force Base in Mississippi, USA (MADE 1). The simulation addresses two aspects: (1) comparison of steady and unsteady groundwater flow and the effect on plume spreading, and (2) analysis of the effects of uncertainty on the hydraulic conductivity map on simulation results. Simulation of the MADE1 experiment shows that small variations in the gradient have no significant impact on the aquifer response and transport of solutes. However, temporal variations in the magnitude of the gradient coupled with aquifer heterogeneity do account for a substantial part of the lateral spreading of the plume. Poor agreement between the simulations and the MADE1 results can certainly be attributed to the aquifer characterisation. The distributions of the hydraulic conductivity were estimated at a very coarse scale. The depth-averaged maps and the kriged map at elevation of 59m did not enable an accurate simulation because of the lack of data about fine-scale heterogeneity. This may explain why the simulated solute is small compared to the spreading observed in the field.

1 INTRODUCTION

A large-scale natural gradient experiment MADE-1 (MAcroDispersion Experiment-1) has been conducted from October 1986 to June 1988 in a heterogeneous alluvial aquifer with the intent of providing a database for groundwater solute transport model validation. Similar databases are available from the Borden Site (Freyberg, 1986; Sudicky, 1986) and the Cape Cod site (Leblanc et al., 1991; Garabedian et al., 1991). The MADE site is particularly interesting for its heterogeneity. The MADE data have been analysed in a series of papers (Boggs et al., 1992; Adams & Gelhar, 1992; Rehfeldt et al., 1992). Validation of theories and models based on the MADE-1 test are given by Rehfeldt & Gelhar (1992), Zheng and Jiao (1998) and Eggleston & Rojstaczer (1998). The simulation in the present paper is based on data supplied by the papers mentioned above.

2 SITE DESCRIPTION

The site is located at the Columbus Air Force Base in Mississippi (see Figure 1 left). The unconfined shallow aquifer is an alluvial terrace deposit averaging 11m of thickness: the aquifer is composed of poorly sorted to well-sorted sandy gravel and gravely sand with minor amounts of silt and clay. Marine sediments consisting of clay, silts and fine-grained sand form a semi-pervious layer (aquitard) beneath the aquifer (Boggs et al., 1992).

The hydraulic head has been monitored with a network of piezometers. At the location of the tracer test the head exhibits a complex temporal and spatial variability produced by the heterogeneity of the aquifer and the large seasonal fluctuations of the water table. Hydraulic conductivities have been derived from 2187 borehole flowmeter measurements. Near the injection point the mean hydraulic conductivity is approximately 10^{-3} cm/s, whereas far from the injection point the conductivities are 1 or 2 orders of magnitude larger. These trends are consistent with the flowmeter measurements of hydraulic conductivity (Boggs, et al., 1992). The aquifer parameters used in this paper are listed in Table 1. Note that these are estimated values and thus represent a source of uncertainty.

Table 1. Aquifer properties.

Parameter	Value
Porosity	0.35
Aquifer thickness	10 m
Specific yield *	0.04 to 0.1
Head gradient	0.003

* Significant uncertainty

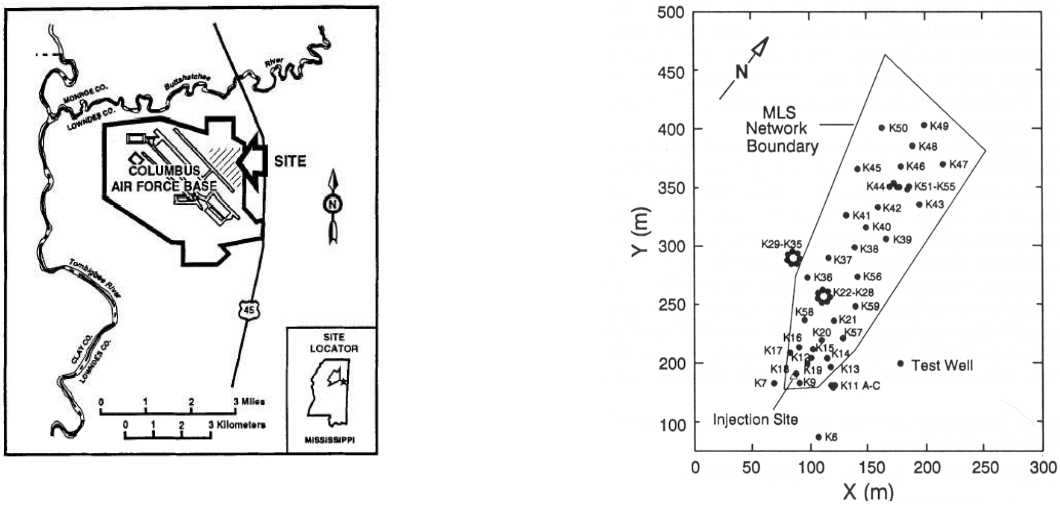

Figure 1. Location of the MADE site (left) and borehole flowmeter measurements (right) (After Boggs et al., 1992).

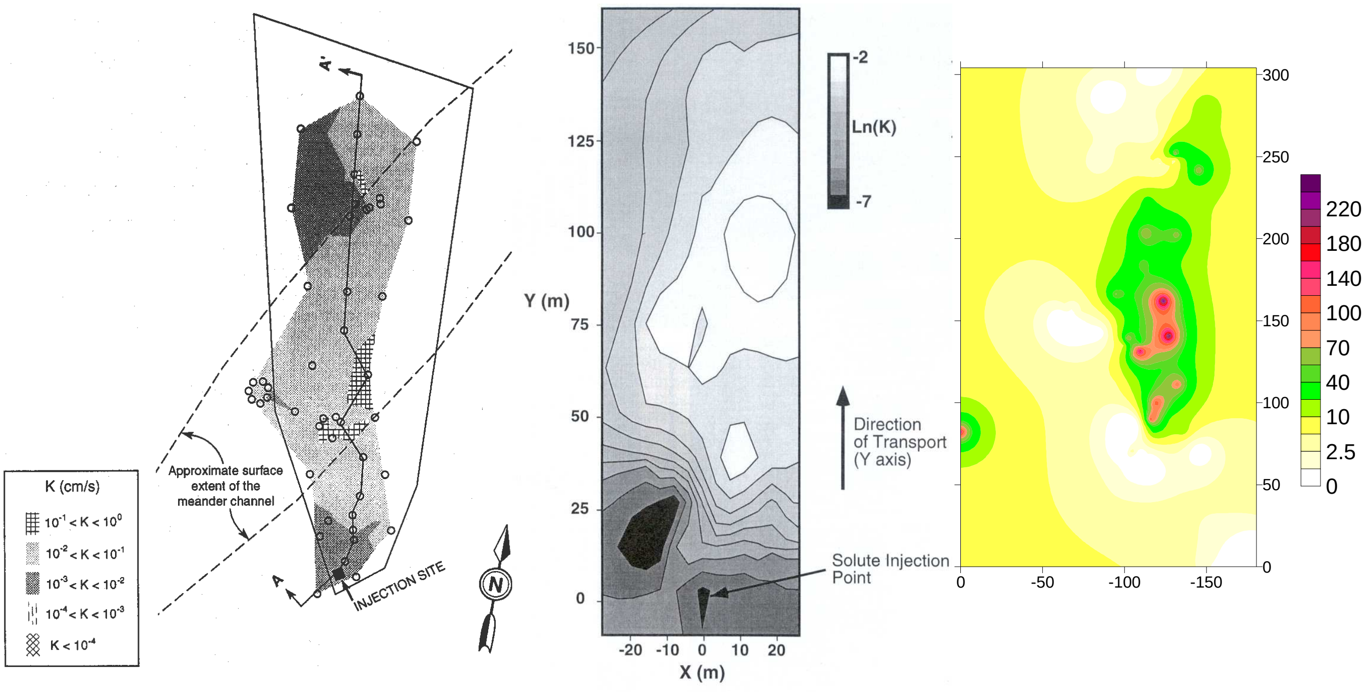

Figure 2. Left: depth-averaged hydraulic conductivity distribution based on borehole flowmeter measurement modified from Boggs et al. 1990 (from Zheng & Jiao, 1998). Middle: Kriged map of the depth-averaged natural log of hydraulic conductivity in the upper part of the aquifer (from Harvey & Gorelick, 2000). Right: Kriged map at depth of 59 m based on raw data from Harvey (2003).

Figure 2 shows a map of the depth-averaged hydraulic conductivity, a kriged map of the depth-averaged log of the hydraulic conductivity in the upper part of the aquifer (from Harvey & Gorelick, 2000) and a kriged map for a depth of 59 m based on raw data from Harvey (2003).

The seasonal fluctuations in the horizontal head gradient as measured in October 1989 at the MADE1 site are presented in Figure 3. Iso-concentration plots of the vertically averaged bromide concentration are presented in Figure 4. Concentrations are plotted at 49, 279 and 503 days after injection. The main feature of the plume is the asymmetry of the concentration distribution in the longitudinal direction: most of the tracer remains close to the injection point, while the front of the plume reaches a distance of more than 160m after 503 days. The horizontal lateral spreading was relatively small and symmetrical.

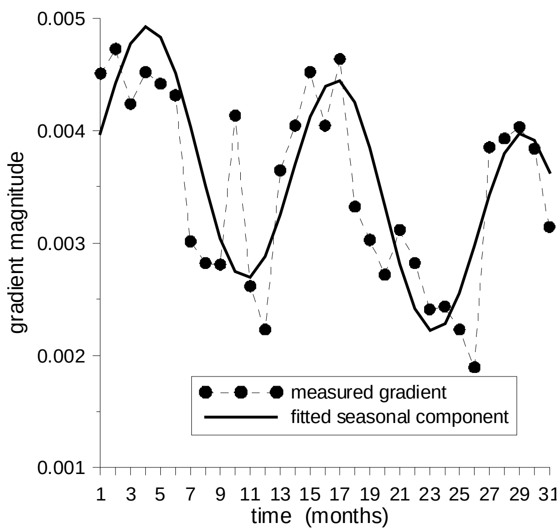

Figure 3. Time series of the magnitude of the hydraulic head gradient at the MADE-1 site (from Rehfeldt & Gelhar, 1992): the field experiment starts in October 1986, i.e. the 17th month.

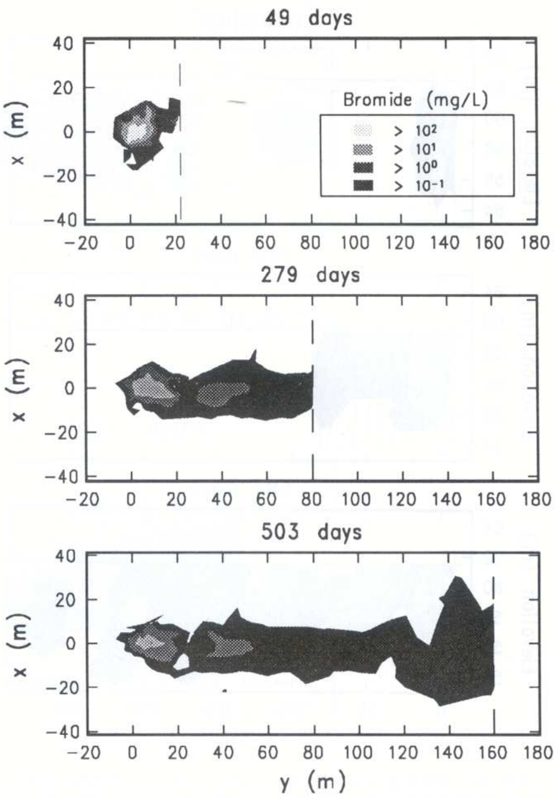

Figure 4. Depth-averaged bromide concentration distributions at 49, 279, and 503 days after injection. Beyond the vertical dashed line, data are missing due to the size of the sampling network (from Boggs et al., 1992).

3 NUMERICAL SIMULATION

3.1 *Velocity distribution*

The flow field (velocity field) has been calculated based on various conductivity maps. The range of conductivity values is presented in Table 2.

Table 2. Range of conductivities from various sources in the literature and this study.

Reference	Conductivity Values
Zheng & Jiao (1998)	0.04- 432 m/day
Harvey & Gorelick (2000)	0.78-117 m/day
Kriging (this study)	0.05- 311 m/day

After a large number of simulations no satisfying results were found and it was concluded that the depth-averaged hydraulic conductivity data from the maps given earlier are too coarse and represent only the large scale heterogeneity. Therefore, a third map has been generated to provide a more accurate representation of the aquifer. By observing the vertical cross-section of the hydraulic conductivity it was found that the plume is injected in a zone of very low permeability (10^{-3}-10^{-4}cm/s). This feature is not reproduced at all in the map of Zheng & Jiao (1998). Moreover it was observed on the vertical cross section of the tracer plume that the plume travels at an averaged elevation 59 m and with a kind of symmetry around this level. Therefore, only values of K at elevation 59 m were used to generate this new map.

3.2 *Tracer experiment*

Simulation solute transport was performed first under steady state conditions. A constant hydraulic head gradient 0.003 was assumed between the upstream and the downstream boundary. Head contours are presented in Figure 5 and are compared with the head contours observed during the MADE-1 experiment (one of the simulated head field is displayed with contours filled with colours, otherwise contour labels can’t appear clearly on the figure).
The distribution of head contours is quite satisfying. Near the injection point the head contours are closely spaced and in the far field, they are widely spaced. The most realistic map seems to be the spatial distribution of K at elevation 59-m, which gives results very close the head field from deep observation wells.

3.2.1 *Steady flow conditions*

In the test site, a conservative tracer was used to study physical transport processes. A bromide tracer in a form of $CaBr_2$ was used as the primary tracer and three fluorobenzoates as secondary tracers (FBA). The tracers have been injected as a uniform pulse approximately at the middle of the saturated zone with a minimal amount of disturbance to the natural flow field. A volume of 10.07 m^3 of groundwater containing 2500 mg/L of bromide and 400 mg/L of each of the FBA tracers was injected at

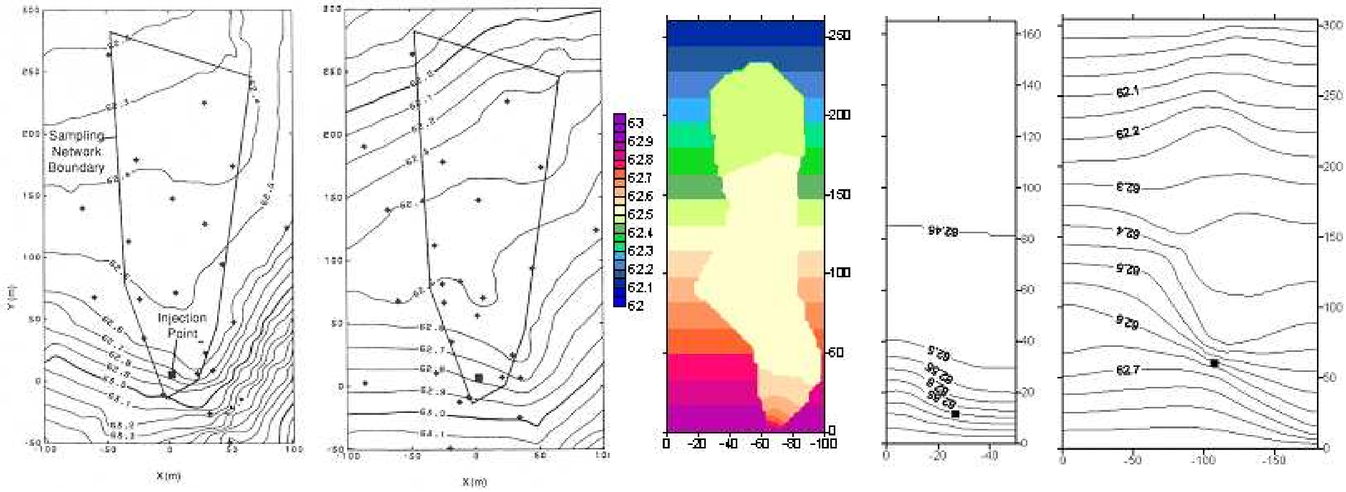

Figure 5. Observed and simulated head contours. Left two images are head contours from shallow and deep observation wells respectively. 3rd and 4th images from left and right images are simulated head contours derived from data from Zheng & Jiao (1998), Harvey & Gorelick (2000), and kriged map at elevation 59m respectively

a uniform rate over a period of 48.5 hours through five wells spaced 1 m apart in a linear array.

The monitoring method is multilevel samplers (MLS) to provide water samples from discrete zones in the aquifer. Data available from the papers are concentration maps represented in the vertical cross-section and also vertically averaged bromide plumes. In the current study, focus is put on the horizontal concentration maps available at 49, 279, 503 days after injection and observed plume characteristics available at several dates (Figure 4, previous section). Parameters used for the solute transport simulation are reported in Table 3.

Table 3. Transport simulation parameters under steady state.

Parameter	Value
Head gradient	0.003
Injected mass	25 kg
Size of the source	0.1 m $\times$ 4 m
Number of particles	100 000
Time step	1 day

For the hydraulic conductivity three different distributions have been assumed referred to below as case 1, case 2 and case 3. For each case a simulation is performed using small values for the dispersivities (α_L = 0.1 m, α_T = 0.01 m) and one using large values (α_L = 1 m, α_T = 0.5 m).

Case 1: Distribution K by Zheng & Jiao

Plots of plume concentrations are given in Figure 6. For small dispersivities, almost no spreading of the plume occurs. The concentration remains beyond 100mg/L. With large dispersivities, more spreading is observed and the tracer is more diluted. At t = 500 days or more, the tracer begins to discharge into the area with higher hydraulic conductivity. However, neither with small nor with large dispersivities the observed plume (Figure 4) is reproduced.

Case 2: Distribution K by Harvey & Gorelick

Plots of plume concentration are presented in Figure 7. The difference with case 1 is that the plume is injected in zone of lower conductivity (0.78m/day). Unfortunately, the plume seems not trapped near the injection like in the observed plume. The tracer goes into zones of higher conductivity and the spreading is also not similar to the observed spreading. With large dispersivities, the extension of the plume is closer to reality (after 500 days, the length of the plume reaches 90m) but the concentration distribution is not satisfying.

Case 3: Distribution K at elevation 59m (present study)

Plots of plume concentrations are given in Figure 8. As in case 2, the plume is injected in a low conductivity zone (≈ 0.60 m/day). The tracer remains near the injection point like in the field test. The conductivity is so low that for small dispersivities, the plume doesn't move. With higher dispersivities the simulated plume is much more similar to the observed one. The extension is not so large (only 70m) but the distribution of concentration is very close to reality. Indeed, 49 days after injection, concentration is more than 100mg/L. Afterwards, there is a dilution of the tracer. The shape and extension of zones of concentration 1 < C < 10 and 10 < C <100 mg/L are better represented.

3.2.2 *Transient flow conditions*

The head gradient at the MADE site fluctuates as shown in Figure 3. Two types of variations are imposed at the downstream boundary: 1) the seasonal component (cosine function) and 2) the measured component (dots) in order to study the difference between large and small-scale temporal variabilities.

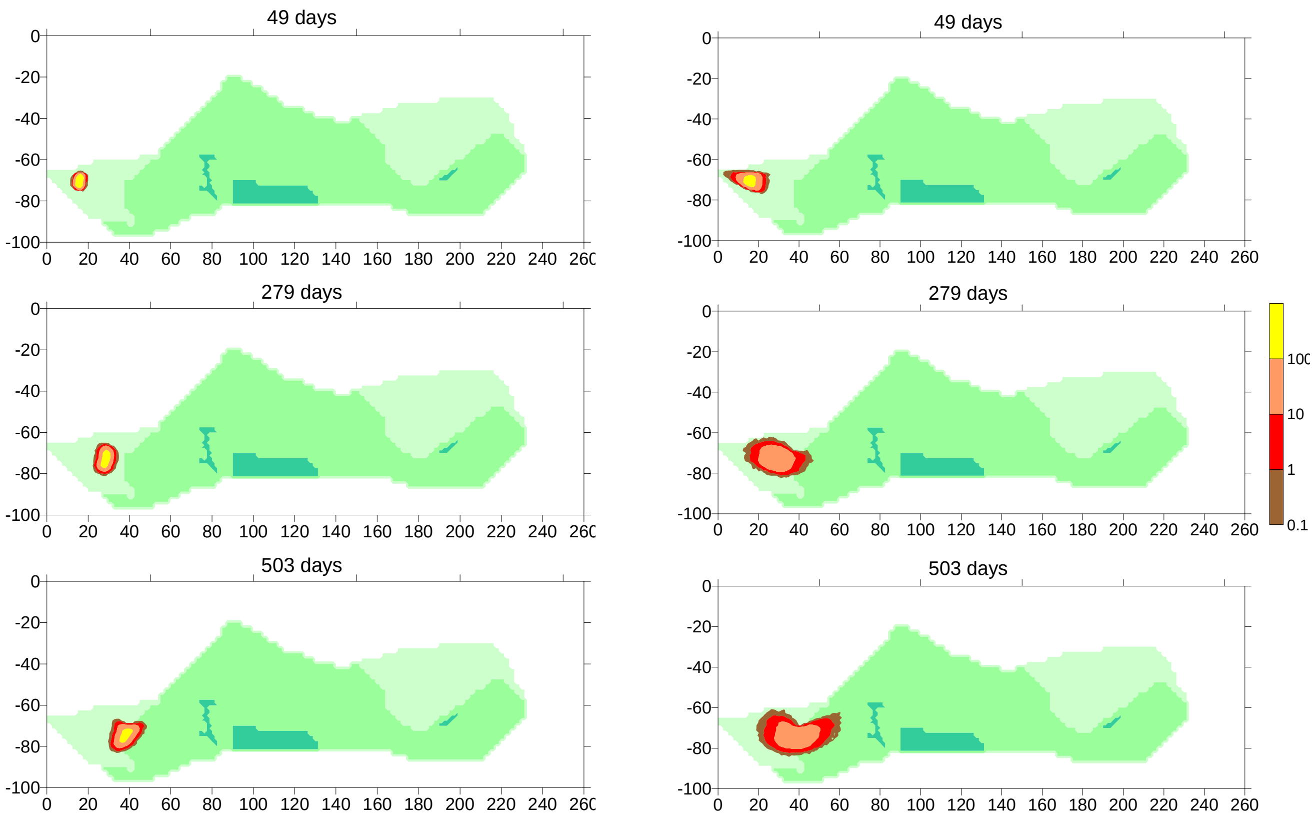

Figure 6. Case 1. Simulation of the bromide tracer test (concentration in mg/L). Left: dispersivities α_L= 0.1 m, α_T = 0.01 m. Right: dispersivities α_L= 1 m, α_T = 0.5 m

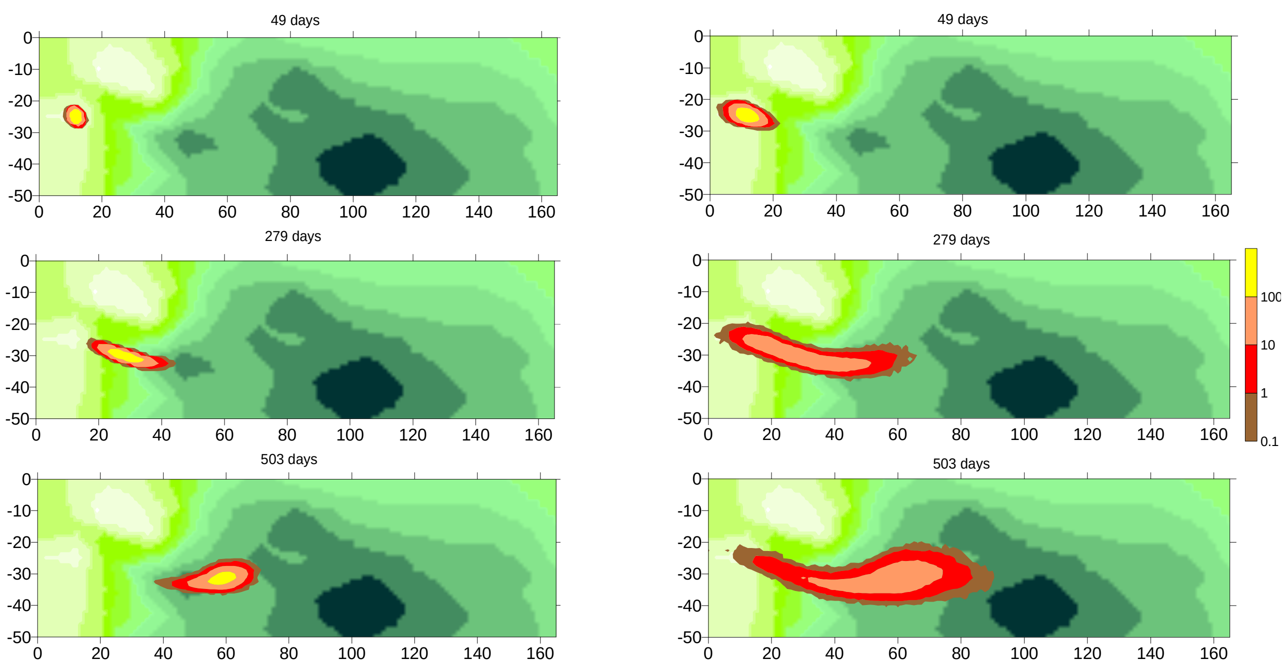

Figure 7. Case 2. Simulation of the bromide tracer test (concentration in mg/L). Left: dispersivities α_L= 0.1 m, α_T = 0.01 m. Right: dispersivities α_L= 1 m, α_T = 0.5 m

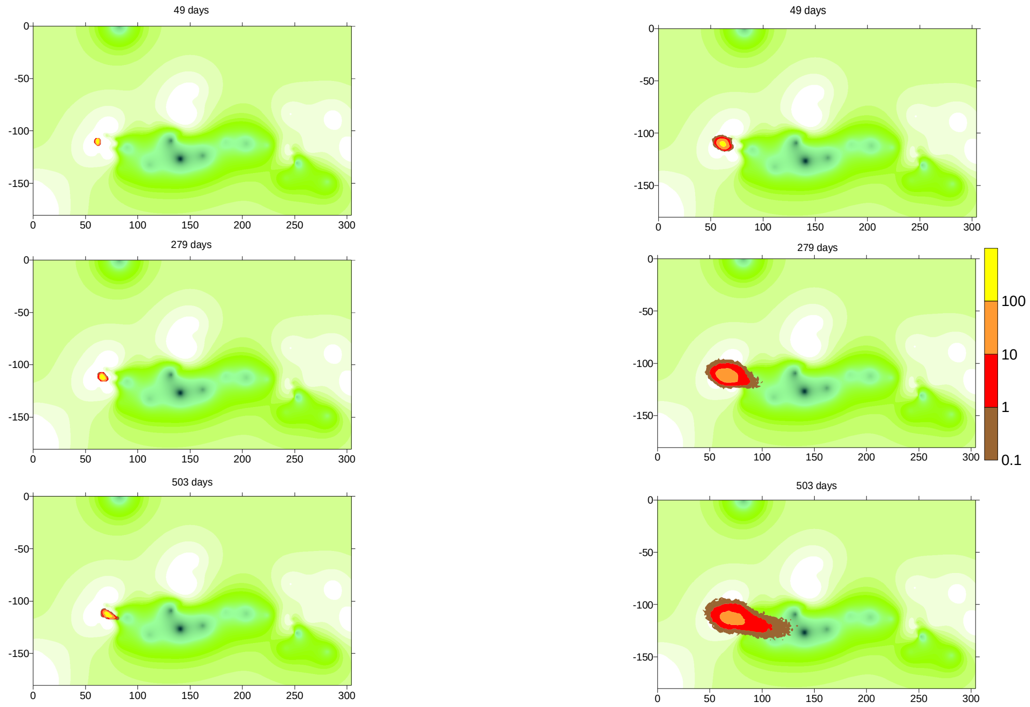

Figure 8. Case 3. Simulation of the bromide tracer test (concentration in mg/L). Left: dispersivities α_L= 0.1 m, α_T = 0.01 m. Right: dispersivities α_L= 1 m, α_T = 0.5 m

From two field tests the storativity of the aquifer was estimated between 0.04 and 0.1. Simulations have been performed for both values. Little difference has been observed between the plume characteristics for S = 0.1 and S = 0.04. Thus, for the simulation with measured variations in the gradient (dots), S = 0.04 has been chosen.

The results for transient flow conditions are similar to the results for steady conditions. Therefore, plumes are not plotted but only spatial moments of the plume (Figures 9-12; from left to right: first moment in x, first moment in y, second centralised moment in x and second centralised moment in y). Simulations with the spatial distribution of K data from Zheng & Jiao (2000) have not been performed, because compared to case 2 and 3 they give no additional information.

4 DISCUSSION

Simulation under transient conditions does not lead to a significant improvement in comparison to the simulation under steady state conditions. Also, temporal variations in the gradient have no significant impact on the plume characteristics, although the lateral spreading shows a small enhancement for the transient case (see Figures 10 and 12). The plume characteristics simulated under the full signal of temporal variability (measured data) does not show significant difference when compared with simulated plumes under only seasonal variability. The agreement between observed and simulated moments is not that good. Our results, in general, underestimate the observed data. Even though the simulated mean displacement is, in general, quite close to reality, it is obvious from the plume plots that it is not representative of the real plume evolution. The displacement of the centre in the y-direction is in the opposite direction: this may be due to the fact that in our simulation we considered fixed boundaries on left and right and we considered only the case of gradient magnitude variability.

The spreading is small compared with the field test results. Our simulation results show a similar trend as in the observed plume. However, the simulated concentrations appear to underestimate the observations. This may be due to the uncertainty in the initial plume size, and in the K distribution, or to our consideration regarding the boundary conditions of the head (case of magnitude variability is only considered). The fact that the observations are depth averaged concentrations, while our simulations are based on depth averaged conductivity map (Zheng & Jiao, 1998 and Harvey & Gorelick, 2000) or in the slice map (this study) may also contribute to this. The best agreement is obtained with the spatial distribution of K at elevation 59m for large dispersivities, except for the longitudinal spreading.

The longitudinal and lateral pore-scale dispersivities were assumed to $\alpha_L = 0.1\,\text{m}$, $\alpha_T = 0.01\,\text{m}$ However, the spreading of the simulated plumes was not satisfying. Values of dispersivities have been increased for a better representation of the plume spreading. By taking larger dispersivity values, we take into account the dispersion that occurs within each grid cell. This dispersion at a finer scale is added to the dispersion that occurs at the scale of the grid (about 1 m).

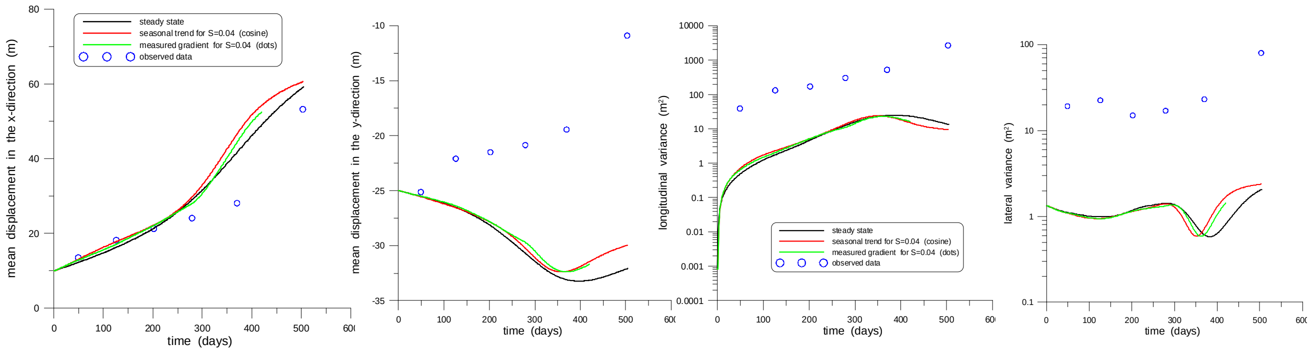

Figure 9. Case 2**.** Spatial moments of the plume for small dispersivities $\alpha_L = 0.1$ m, $\alpha_T = 0.01$ m .

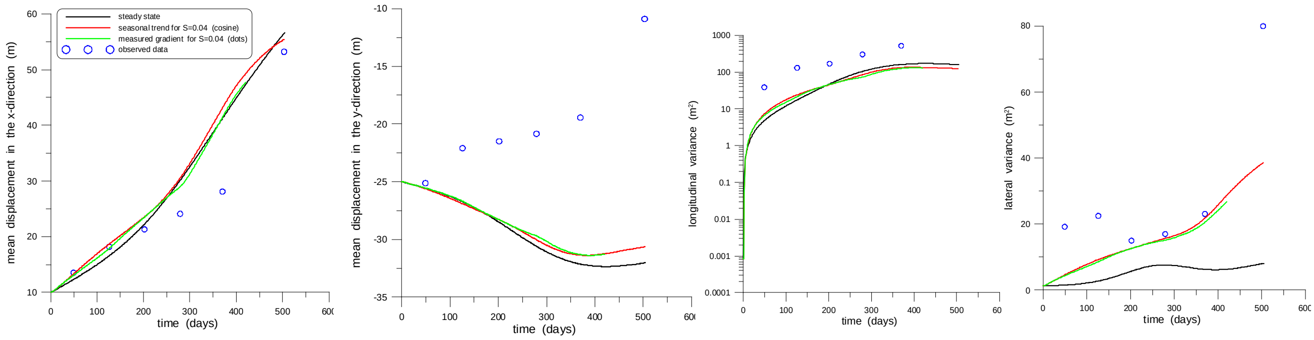

Figure 10. Case 2. Spatial moments of the plume for large dispersivities $\alpha_L = 1$ m, $\alpha_T = 0.5$ m .

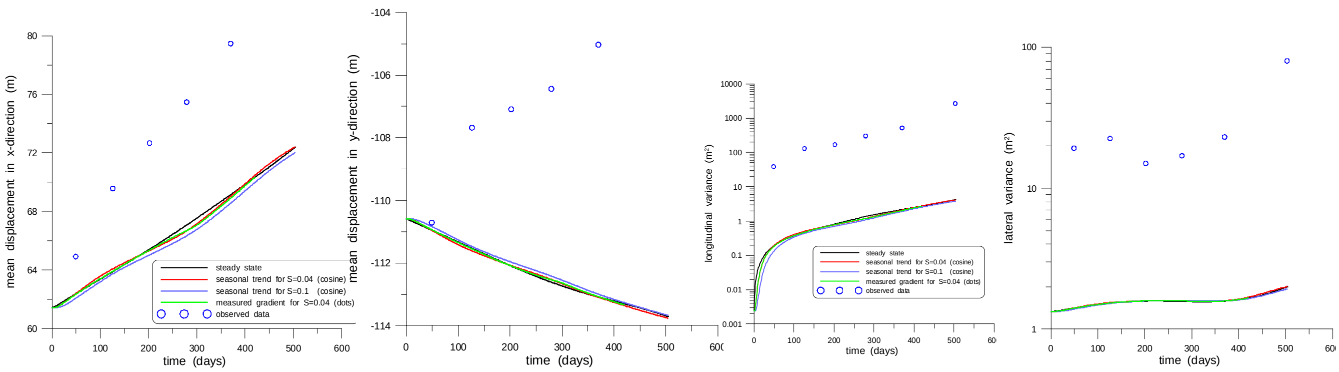

Figure 11. Case 3. Spatial moments of the plume for small dispersivities $\alpha_L = 0.1$ m, $\alpha_T = 0.01$ m .

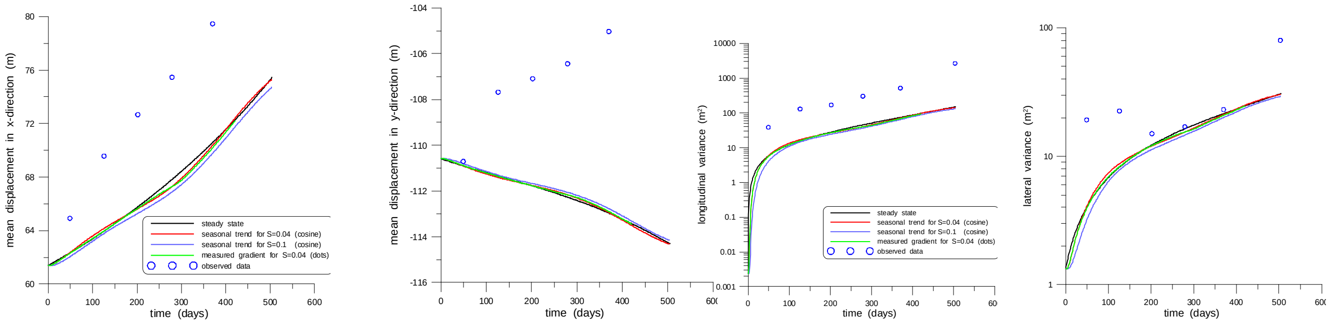

Figure 12. Case 3. Spatial moments of the plume for large dispersivities $\alpha_L = 3$ m, $\alpha_T = 1$ m .

5 CONCLUSIONS

Simulation of the MADE1 experiment has shown that small variations in the gradient magnitude have no significant impact on the aquifer response and the transport of solutes. In our simulations the maximum variation in the gradient magnitude is only about 0.0025. It could be interesting to study transient flow conditions in coastal aquifers, where tides may produce temporal variations with a large amplitude that have significant impact on transport.

Poor agreement between the simulations and the MADE1 results can certainly be attributed to the aquifer characterisation. Indeed the different distributions of K were estimated at a coarse scale. The depth-averaged maps and the kriged map at elevation 59m did not enable to simulate the dispersion process reasonably because of the lack of data about fine-scale heterogeneity. This can explain why the spreading in our simulation is very small compared with spreading in the field test. A good knowledge of the geology and heterogeneity of the aquifer (Eggleston & Rojstaczer, 1998, at a scale less than 10m) is necessary to perform acceptable simulations.

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